

AR201-13949



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Eastman"  
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>

To: NCIC HPV@EPA  
CC:  
Subject: HPV test plan

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2002 SEP 12 PM 12:24

08/30/2002 08:04 AM

Attached is a HPV test plan for C4 aldehydes self condensation products CAS# 68990-21-6. A signed hard copy of the letter and a diskette containing the test plan were mailed on the 29th.

<<Whittman - Solvent C test plan letter.doc>> <<Sovent C (082602).pdf>>

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Whittman - Solvent C test plan letter; Sovent C (082602).pc

August 26, 2002

Ms. Christine Todd Whitman, Administrator  
US EPA  
PO Box 1473  
Merrifield, VA 22116

Attn: Chemical Right-to-Know Program

**RE: HPV Chemical Challenge Program, AR-201**

Dear Ms Whitman:

On behalf of Eastman Chemical Company, I am pleased to submit the test plan and robust summaries for "Aldehydes, C4, self-condensation products, high-boiling fraction (Solvent C; CAS NO.: 68990-21-6). My company had agreed to sponsor this chemical and provide the Agency with the enclosed information in the year 2003. However, due to the substantial amount of data that had been previously generated to understand the potential hazards of this chemical, we were able to complete our summarization ahead of schedule.

Enclosed with this letter is a computer diskette containing the test plan and robust summaries in Adobe Acrobat (.pdf) format. The HPV registration number for Eastman Chemical is

We understand this information will be posted on the internet for comments for a period of 120 days. Please forward comments to me at the above address.

Sincerely,

James A. Deyo D.V.M., Ph.D., D.A.B.T.  
Technical Associate

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AR201-13949A

2002 SEP 12 PM 12: 25

HIGH PRODUCTION VOLUME (HPV) CHALLENGE PROGRAM

TEST PLAN  
FOR  
ALDEHYDES, C4, SELF-CONDENSATION PRODUCTS, HIGH-BOILING FRACTION  
(CAS NO.: 68990-21-6)

PREPARED BY:  
EASTMAN CHEMICAL COMPANY

August 29, 2002

## **TEST PLAN SUMMARY**

The Eastman Chemical Company hereby submit for review and public comment the test plan for aldehydes, C4, self-condensation products, high-boiling fraction (Solvent C; CAS NO.: 68990-21-6) under the Environmental Protection Agency's (EPA) High Production Volume (HPV) Chemical Challenge Program. It is the intent of our company to use existing data already generated on either the constituents of Solvent C or expected metabolites of them in conjunction with EPA-acceptable predictive computer models to adequately fulfill the Screening Information Data Set (SIDS) for the physicochemical, environmental fate, ecotoxicity test, and human health effects endpoints. We believe that the information already available, or in the process of being generated, are adequate to fulfill all the requirements of the HPV program without need for the conduct of any new or additional tests.

Solvent C is essentially manufactured and handled in closed-systems with minimal chance for exposure in the workplace or to the general population. The primary use (approximately 93%) of this product is as a fuel for burning. In this application, product is either shipped by tank truck to other sites within the company where it is burned directly or marketed to a few customers where it is blended at a level of less than 1% into fuel oils used by consumers to burn for home heating. Other minor or occasional uses of this product include its use as a solvent in asphalt production and as part of a process solvent in the industrial extraction of phosphoric acid from rock. This latter end-use is also performed in closed systems. Thus, there is essentially no exposure to this chemical by the general public and in industrial settings, exposure is minimized by how it is manufactured and handled. There are a very limited number of customers using Solvent C with the potential for exposure only manifested during its transfer to and from tank trucks or under conditions of an industrial accident. In total, exposure to Solvent C is very limited in both its potential duration and frequency.

Solvent C is described as a yellow-green liquid. It is a Class 2 chemical consisting of approximately 10 major chemicals consisting of the CAS registry numbers displayed below in Table 1 and their approximate percentages. Of these 10 major constituents, 7 have already been, or are in the process of being, evaluated through the OECD or ICCA SIDS program, or the US HPV program. Of the remaining three not in a formalized HPV program, one, butyl butyrate, has been approved by the FDA as a synthetic flavoring agent for food under 21CFR 172.515 and is found naturally in many types of fruits. This compound is formed through an ester linkage between n-butanol and butyric acid. It would be expected that this ester linkage would readily be cleaved to yield the parent molecules butyric acid and butanol, both of which are in the ICCA SIDS program. A second nonHPV chemical, 2-ethyl-1,3-hexanediol was at one time registered with the EPA for use as an insect repellent for use by humans and has a history of use in cosmetics and other industrial applications. Thus, significant amounts of toxicity information have already been developed and are available to the public either through the EPA or in peer-reviewed journals. This chemical is only present at a maximum concentration of 10%. Thus, data are currently available for public review on the majority of the chemicals comprising Solvent C with most of this information in summary format. The third nonHPV chemical, di-2-ethylhexyl ether, is listed by the EPA as a Class 3 inert ingredient for use in pesticides. The EPA's Office of Pesticide Programs has contracted a Structure Activity Team (SAT) to prepare toxicological and ecological assessments for these inert ingredients. While there is essentially no mammalian toxicity data identified on it, it is not acutely toxic with a reported LD<sub>50</sub> of 34 gm/kg. Another chemical found within Solvent C is listed as "alkyl acetals". These chemicals comprise a small portion of the total (2-10%) and are formed by a reaction between alcohols and aldehydes. The reaction is readily reversed in the presence of an acid.

In conclusion, Solvent C is a complex mixture of several chemicals. It is manufactured, handled, and marketed into end uses in such a manner that, except under conditions of an accident, exposures are very limited. Hazard assessment information in the form of robust summaries or as published literature for most all the SIDS endpoints are either currently available or will be made publicly available through various ongoing HPV programs. This information adequately characterizes the hazard potential for the majority of the chemical constituents in Solvent C and thus would likely represent the potential hazards of Solvent C. The goal of the HPV program is to have a screening level of understanding of the hazards presented by a chemical available to the public. Eastman believes the data identified to date that are presently available to the EPA and the general public, in total, fulfill this objective and that further toxicity studies would not be warranted on a chemical mixture whose constituents vary and has such low potential for human exposure. Accordingly, Eastman believes that the obligations of our commitment to this chemical in the HPV challenge program have been completed through this submission.

**Table 1 - Solvent C (CAS No.:68990-21-6)**

2002 SEP 12 PM 12: 25

Cas No.	Chemical	Composition Percentage	General Comments
10143-60-9	di-2-Ethylhexyl ether	25-35	The only data located was an LD50 that indicates it is of low toxicity (LD <sub>50</sub> of 33.9 g/kg; Smyth, H.F., 1954). It is listed by the EPA as a Class 3 inert ingredient for use in pesticide formulations. The EPA is in the process of preparing toxicological and ecological assessments for this class level of inert ingredients.
109-21-7	Butyl butyrate	8-16	Material is an FDA-approved food flavorant and is naturally present in many types of fruits. It is fully expected to metabolize to butyric acid and n-butanol in mammals. Both these chemicals are in the ICCA HPV program.
126-30-7	Neopentyl glycol	7-11	An OECD/SIDS assessment has been completed.
144-19-4	2,2,4-Trimethyl-1,3-pentanediol	7-11	A complete test plan with robust summaries for all end points has been submitted into the EPA as part of the HPV program.
71-36-3	n-butyl alcohol	5-10	Material is in the ICCA/SIDS program.
94-96-2	2-Ethyl-1,3-hexanediol	5-10	Material has been thoroughly characterized for use as an insect repellant for human uses. Although its registration has been cancelled, essentially all SIDS data are available through published literature.
NA	Alkyl Acetals	2-10	Formed by a reaction between alcohols and aldehydes. The reaction is readily reversed in the presence of an acid.
104-76-7	2-Ethylhexanol	4-6	An OECD/SIDS assessment has been completed.
78-83-1	Isobutyl alcohol	2-6	Material is in the ICCA/SIDS program.
97-85-8	Isobutyl isobutyrate	2-6	Material is in the ICCA/SIDS program.
107-92-6	Butyric acid	1-2	Material is in the ICCA/SIDS program.

#### **SIDS DATA SUMMARY**

Solvent C is a mixture of several chemicals, the majority of which have already been or are in the process of being evaluated in the OECD SIDS program, the ICCA SIDS program, or the US EPA HPV program. Accordingly, it should be assumed that they already have or will have complete data sets and have robust summaries available as a result of their participation in these programs. Another chemical, 2-ethyl-1,3-hexanediol, present at a level of 5-10% has data assessing all of the mammalian endpoints available to the public via peer-reviewed journals. This is the only other chemical with significant amounts of data that can be used to assist in determining the hazard potential of the mixture. However, since it only constitutes a small fraction of the total its toxicity is not likely to impact the overall toxicity in a significant manner and all data available indicate it is of low toxicity to both mammalian and environmental species. Since Solvent C consists of many chemicals present in varying amounts it is not known how the various SIDS endpoints will be affected by their presence as a mixture. Due to the fact that the actual percentage of each chemical can vary, Eastman believes there would be little value in conducting any new animal studies on Solvent C when the hazard associated with the majority of its constituents have been already assessed.

**PHYSICAL CHEMICAL DATA**

Cas No.	Chemical	Melting Point*	Boiling Point	Vapor Pressure	Partition Coefficient	Water Solubility
10143-60-9	di-2-Ethylhexyl ether	NA	X	X	X	X
109-21-7	Butyl butyrate	NA	X	X	X	X
126-30-7	Neopentyl glycol	NA	X	X	X	X
144-19-4	2,2,4-Trimethyl-1,3-pentanediol	NA	X	X	X	X
71-36-3	n-butyl alcohol	NA	X	X	X	X
94-96-2	2-Ethyl-1,3-hexanediol	NA	X	X	X	X
NA	Alkyl Acetals	NA				
104-76-7	2-Ethylhexanol	NA	X	X	X	X
78-83-1	Isobutyl alcohol	NA	X	X	X	X
97-85-8	Isobutyl isobutyrate	NA	X	X	X	X
107-92-6	Butyric acid	NA	X	X	X	X

\* Material is a liquid at room temperature

Data for these endpoints can be found within the various SIDS documents already drafted or in the process of being developed for the OECD, ICCA or US EPA HPV programs. In addition, data are available through the use of computer estimation modeling programs (EPIWIN) that are available to the public.

**ENVIRONMENTAL FATE**

Cas No.	Chemical	Photo-degradation	Water Stability	Biodegradation	Fugacity
10143-60-9	di-2-Ethylhexyl ether	X			X
109-21-7	Butyl butyrate	X	X		X
126-30-7	Neopentyl glycol	X	X	X	X
144-19-4	2,2,4-Trimethyl-1,3-pentanediol	X	X	X	X
71-36-3	n-butyl alcohol	X	X	X	X
94-96-2	2-Ethyl-1,3-hexanediol	X	X	X <sup>1</sup>	X
NA	Alkyl Acetals				
104-76-7	2-Ethylhexanol	X	X	X	X
78-83-1	Isobutyl alcohol	X	X	X	X
97-85-8	Isobutyl isobutyrate	X	X	X	X
107-92-6	Butyric acid	X	X	X	X

Data for these endpoints can be found within the various SIDS documents already drafted or in the process of being developed for the OECD, ICCA or US EPA HPV programs. In addition, data are available through the use of computer estimation modeling programs (EPIWIN) that are available to the public.

- 1.) Data (OECD 301E and 302B) listed in a MSDS from Dixie Chemical Company, Inc. Houston, TX indicate this material is readily degradable.

## ECOTOXICITY DATA

Cas No.	Chemical	Fish Toxicity	Daphnia Toxicity	Algae Growth Inhibition
10143-60-9	di-2-Ethylhexyl ether			
109-21-7	Butyl butyrate	X <sup>1</sup>		
126-30-7	Neopentyl glycol	X	X	X
144-19-4	2,2,4-Trimethyl-1,3-pentanediol	X	X	X
71-36-3	n-butyl alcohol	X	X	X
94-96-2	2-Ethyl-1,3-hexanediol	X <sup>2</sup>	X <sup>2</sup>	
NA	Alkyl Acetals			
104-76-7	2-Ethylhexanol	X	X	X
78-83-1	Isobutyl alcohol	X	X	X
97-85-8	Isobutyl isobutyrate	X	X	X
107-92-6	Butyric acid	X	X	X

Data for these endpoints can be found within the various SIDS documents already drafted or in the process of being developed for the OECD, ICCA or US EPA HPV programs. In addition, data could be generated through the use of computer estimation models that are available to the public.

- 1.) Curtis, M.W. and Ward C.H. (1981). Aquatic Toxicity of Forty Industrial Chemicals: Testing in Support of Hazardous Substance Spill Prevention Regulation. *J Hydrology*, **51**, 359-367.
- 2.) Data (LC0(48hr) Fish > 1000 mg/L; EC50(24 hr) Daphnia 811 mg/L) listed in a MSDS from Dixie Chemical Company, Inc. Houston , TX

## TOXICOLOGICAL DATA

Cas No.	Chemical	Acute Toxicity	Repeat Dose Toxicity	Genotoxicity Mut./Aberr.	Developmental Toxicity	Reproductive Toxicity
10143-60-9	di-2-Ethylhexyl ether	X <sup>1</sup>				
109-21-7	Butyl butyrate	X <sup>2</sup>	X <sup>3</sup>	X/X <sup>3</sup>	X <sup>3</sup>	X <sup>3</sup>
126-30-7	Neopentyl glycol	X	X	X/X	X	X
144-19-4	2,2,4-Trimethyl-1,3-pentanediol	X	X	X/X	X	X
71-36-3	n-butyl alcohol	X	X	X/X	X	X
94-96-2	2-Ethyl-1,3-hexanediol	X <sup>4</sup>	X <sup>5,6</sup>	X/X <sup>7</sup>	X <sup>8</sup>	X <sup>5,6</sup>
NA	Alkyl Acetals					
104-76-7	2-Ethylhexanol	X	X	X/X	X	X
78-83-1	Isobutyl alcohol	X	X	X/X	X	X
97-85-8	Isobutyl isobutyrate	X	X	X/X	X	X
107-92-6	Butyric acid	X	X	X/X	X	X

Data for these endpoints can be found within the various SIDS documents already drafted or in the process of being developed for the OECD, ICCA or US EPA HPV programs.

1. Smyth, H.F. (1954). Range-Finding Toxicity Data: List V. *AMA Arch. Ind. Hyg. Occup. Med.* **10**, 61-68.
2. Butyl n-butyrate: Fragrance raw materials monographs. *Food Cosmetics Toxicology* **17**, 521-522 (1979); RTECS Number: ES8120000
3. Endpoint evaluated through use of surrogates butyric acid and n-butanol
4. Ballantyne, B. (1985). The Acute Toxicity and Primary Irritancy of 2-Ethyl-1,3-Hexanediol. *Vet. Hum. Toxicol.* **27(6)**, 491-495.
5. VanMiller, J.P., *et al.* (1995). Repeated Exposure Toxicity of 2-Ethyl-1,3-Hexanediol by Cutaneous Applications to the Rat for 9 and 90 Days. *Vet. Hum. Toxicol.* **37(1)**, 33-36.
6. Stenback, F. and Shubik, P. (1974). Lack of Carcinogenicity of Some Commonly Used Cutaneous Agents. *Toxicol. Appl. Pharmacol.*, **30**, 7-13.
7. Slesinski, R.S., *et al.*, (1988). In Vitro and In Vivo Evaluation of the Genotoxic Potential of 2-Ethyl-1,3-Hexanediol. *Toxicology*, **53(2-3)**, 179-198.
8. Neeper-Bradley, T.L., *et al.* (1994). Evaluation of the Developmental Toxicity Potential of 2-Ethyl-1,3-Hexanediol in the Rat by Cutaneous Application. *J. Toxicol. – Cut. & Ocular Toxicol.*, **13(3)**, 203-214.